

Dynamical local field, compressibility, and frequency sum rules for quasiparticles

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The finite temperature dynamical response function including the dynamical local field is derived within a quasiparticle picture for interacting one-, two-, and three-dimensional Fermi systems. The correlations are assumed to be given by a density-dependent effective mass, quasiparticle energy shift, and relaxation time. The latter one describes disorder or collisional effects. This parametrization of correlations includes local-density functionals as a special case and is therefore applicable for density-functional theories. With a single static local field, the third-order frequency sum rule can be fulfilled simultaneously with the compressibility sum rule by relating the effective mass and quasiparticle energy shift to the structure function or pair-correlation function. Consequently, solely local-density functionals without taking into account effective masses cannot fulfill both sum rules simultaneously with a static local field. The comparison to the Monte Carlo data seems to support such a quasiparticle picture.

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I. INTRODUCTION

The response of an interacting Fermi system with the potential V_q to an external perturbation is the basic source of our knowledge about the interaction, and dynamical as well as static properties of the system. This response function has been therefore a central issue of many-body theories.

The density response function gives the variation of the density in terms of the external potential,

$$\delta n(q, \omega) = \chi(q, \omega) V^{\text{ext}}(q, \omega). \quad (1)$$

The polarization is defined as the density variation in terms of the induced potential,

$$\delta n(q, \omega) = \Pi(q, \omega) \delta V^{\text{ind}}(q, \omega), \quad (2)$$

where we suppress the notation of obvious q dependence in the following. The induced potential itself is the sum of the external potential and the effective interaction potential, $[V_q + f_q(\omega)] \delta n$,

$$\delta V^{\text{ind}}(\omega) = [V_q + f_q(\omega)] \delta n(\omega) + V^{\text{ext}}(\omega). \quad (3)$$

Therefore, from Eqs. (1)–(3) we have the relation between response and polarization,

$$\chi(\omega) = \frac{\Pi(\omega)}{1 - [V_q + f_q(\omega)] \Pi(\omega)}. \quad (4)$$

The local field $f_q(\omega)$ describes the modification in the restoring force brought about by particle correlations. This field prevents the particles from sampling the full effect of interaction at short distances.¹

The dielectric function relates now the induced densities to the external potential via

$$\frac{1}{\epsilon(\omega)} = 1 + \frac{V_q \delta n(\omega)}{V^{\text{ext}}(\omega)} \equiv 1 + V_q \chi(\omega), \quad (5)$$

such that the dielectric function reads

$$\epsilon(\omega) = 1 - \frac{V_q \Pi(\omega)}{1 - f_q(\omega) \Pi(\omega)}. \quad (6)$$

The theoretical effort consists in determining the local field $f_q(\omega)$ which represents the local correlation and which depletes the induced potential as $f_q(\omega) = -G(\omega) V_q$. As long as this local field is a dynamical one this is an exact relation. The different theoretical treatments differ in this local-field correction; for an overview see Ref. 2. Mostly static approximations, $f_q \equiv f_q(0) = -V_q G$, have been proposed in the past. It has started with the pioneering work of Hubbard,³ who first introduced the notation of local field and took into account the exchange-hole correction resulting in

$$G_H = \frac{1}{2} \frac{q^2}{q^2 + k_f^2} = \begin{cases} \frac{1}{2} \frac{q^2}{k_f^2} + o(q^3) \\ \frac{1}{2} + o(1/q^2). \end{cases} \quad (7)$$

While this expression has established a remarkable improvement of the dielectric function in the random-phase approximation (RPA), it has been soon recognized insufficient due to the lack of self-consistency, which leads the pair correlation function still to unphysical negative values. This has been repaired by Singwi, Tosi, Land, and Sjölander (STLS)⁴ by using exchange correlations,

$$G_{STLS} = -\frac{1}{n} \int \frac{dk}{(2\pi)^3} \frac{(kq)}{k^2} (S_{k-q} - 1) = \begin{cases} \frac{\gamma q^2}{k_f^2} + o(q^3) \\ 1 - g_0 + o(1/q^2) \end{cases} \quad (8)$$

with

$$\gamma = -\frac{1}{s k_f} \int_0^\infty dq (S_q - 1), \quad (9)$$

where s is the spin degeneracy and where the static structure factor

$$S_q = - \int \frac{d\omega}{n\pi V_q} \frac{\text{Im} \epsilon^{-1}(\omega)}{1 - e^{-\beta\omega}}$$

$$= \int \frac{d\omega}{n\pi} \frac{1}{1 - e^{-\beta\omega}} \text{Im} \frac{\Pi(\omega)}{1 - [f_q(\omega) + V_q]\Pi(\omega)}, \quad (10)$$

where the inverse temperature $\beta = 1/T$ is linked to the pair correlation function via

$$g_r - 1 = \frac{1}{n} \int \frac{dq}{(2\pi)^3} e^{iqr} (S_q - 1). \quad (11)$$

This provides a self-consistent problem in solving the dielectric function, structure function, and static local field simultaneously. The advantages of this result compared to the Hubbard result with respect to the pair-correlation function and large-wave-vector limit have been discussed in Ref. 5. Recent comparisons with molecular-dynamics simulations for a hard-sphere gas are presented in Ref. 6, where a good agreement is found for thermodynamical properties.

The expression (8) has been improved further by Pathak and Vashishta⁷ (PV) demanding that the response function should fulfill the third-order frequency sum rule,⁸ which resulted in

$$G_{PV} = - \frac{1}{n} \int \frac{dk}{(2\pi)^3} \frac{(kq)^2}{q^4} \frac{V_k}{V_q} (S_{k-q} - S_k)$$

$$= \begin{cases} \frac{2}{5} \gamma \frac{q^2}{k_f^2} + o(q^3) \\ \frac{2}{3} (1 - g_0) + o(1/q^2) \end{cases} \quad (12)$$

leading to the improved small-distance limit discussed in Ref. 9. The difference at short distance in G_{STLS} comes from the motion of particles inside the correlation hole, which is condensed in the dynamical behavior.¹⁰

If one takes into account the difference between uncorrelated and correlated kinetic energies^{11,1} one obtains an additional $-\Delta E = -(2/n^2 V_q)(E_{int} - E)$ term in G_{PV} . This comes from the difference between correlated and uncorrelated occupation numbers, which can be expressed by a coupling-constant integration and can be linked via the virial theorem to density derivatives of the pair-correlation function.^{12,13}

Parallel to the above discussions there have been different improvements to the derivation of local fields from the virial formula,^{9,11,14} which have resulted in expressions known from density variations,

$$G_{VS} = \left(1 + an \frac{\partial}{\partial n} \right) G_{STLS}, \quad (13)$$

with various $1/2 \leq a \leq 1$, see Ref. 14. This procedure satisfies the compressibility sum rule almost exactly.

In Ref. 11 it was shown for Coulomb systems that one cannot construct a static local field factor which fulfills both limits, the compressibility and the third-order sum rule (32),

since it would violate the theorem of Ferrell, $d^2 E_0 / d(e^2)^2 \leq 0$. The same conclusions are obtained in Ref. 15 using the virial theorem.

Therefore the concentration is now mostly focused on the construction of dynamical local-field corrections.^{13,16-18} The quantum versions of the Singwi-Tosi-Land-Sjölander, G_{STLS} , and Vashishta-Singwi, G_{VS} , theories have been discussed in Refs. 16, 19, and 20. These lead to positive values for the pair distribution function at short distances valid for rather low densities.¹⁶ There the dynamical properties of the dynamic local field have been focussed upon. While the high-frequency limit is monotonic and similar to STLS and VS, the static limit can even exhibit peaked structures which can give rise to charge-density waves underlying the non-trivial character of the dynamical behavior. Unfortunately, even the dynamic quantum version of the Singwi-Tosi-Land-Sjölander local field cannot fulfill the compressibility sum rule.²¹ We will show here that from a dynamical local field, one can derive a static local field fulfilling both sum rules simultaneously if one takes into account the effective mass. This will resolve the puzzle of sum rules.

Recent improvements in the response function have been basically due to numerical studies of Monte Carlo²²⁻²⁵ or molecular-dynamical simulations.^{26,6} An interesting first-principles numerical scheme is to solve the time-dependent Kadanoff and Baym equations including an external field.²⁷ Due to the variation of internal lines, already a Born diagram leads to a linear response which includes high-order vortex corrections fulfilling sum rules consistently. The third-order frequency sum rule regains importance for reduced-dimensional layered structures.^{25,28,29} All results in this paper here can be straightforwardly generalized also to reduced dimensions as given in Appendix B for one, two, and three dimensions. This could have an impact on recent discussions of two-layered electron gasses.³⁰⁻³²

Here we want to return to the analytical investigations and will show that there exists a possibility to fulfill with one static local-field correction both requirements, the third-order sum rule and the compressibility sum rule. This is performed by working within a quasiparticle picture determining the effective mass appropriately. Within the frame of the quasiparticle picture we will derive an explicit expression for the dynamical local-field factor, which leads to the desired static limits. We obtain the identity

$$G = G_{PV} + \frac{2}{n^2 V_q} (E - E_{int})$$

$$= - \frac{1}{V_q} \left[\frac{\partial \Delta}{\partial n} - \frac{1}{2nm} \frac{\partial \ln m}{\partial \ln n} \left(\frac{\Pi_2(0)}{\Pi_0(0)} - \frac{q^2}{4} \right) \right] \quad (14)$$

with the moments of polarization given in Appendix B and the effective mass $m(n)$ and self-energy $\Delta(n)$. It will provide a way to construct a quasiparticle picture by the knowledge of the structure factor at small distances from experiments or simulations.^{26,22,6} This in turn leads to an easy microscopic parametrization in terms of the effective mass and quasiparticle energy shift, which could be compared directly to microscopic theories.

The underlying principle is analogous to that found in literature,^{33,34} where a response function was parametrized explicitly fulfilling sum rules and different constraints. Other parametrizations can be found in Ref. 13 from variational approaches which are exact in the high-density limit. A different line of constructing the response function uses the frequency moments resulting in recurrence relations.^{35,36}

Here in this paper we will give an alternative approach which uses general parametrizations of the self-energy in terms of a functional that might depend on the density, energy, and current. We restrict here to a one-component system, though the generalization to multicomponent systems is straightforward^{37,38} and is considered in different approaches.^{39–41}

In the following section we review briefly the compressibility sum rule and the third-order frequency sum rule. In Sec. III we give the dynamical response for quasiparticles, which is a special case of the general structure derived earlier.⁴² We show that the correct compressibility appears and the third-order sum rule can be satisfied if the effective mass and quasiparticle energy is chosen appropriately. Section IV will present some numerical results on the unpolarized electron gas at zero temperature, and the comparison with Monte Carlo simulations are discussed. Section V summarizes the results and in Appendix B we give frequently occurring correlation functions and practical forms for the calculation in one-, two-, and three dimensions. While all formulas in the main text are written for three dimensions, they hold for one and two dimensions as well. Only the explicit correlation functions in Appendix B have to be used as outlined there. Also the often required long-wavelength expansion of these correlation functions is given in Appendix B1. Appendix C finally is devoted to a short sketch of the perturbation theory and the derivation of the used sum rules for one, two, and three dimensions.

II. DETERMINATION OF STATIC LOCAL-FIELD FACTOR

Let us discuss two different boundaries for the static limit of the local field. This will be the compressibility and the third-order frequency sum rule.

A. Compressibility

First we have to know how the compressibility should look. This is particularly simple in the quasiparticle picture which we will use. In the quasiparticle picture the one-particle distribution function is a Fermi distribution

$$F(p) = (e^{\beta(p^2/2m + \Delta - \mu)} + 1)^{-1}, \quad (15)$$

where the density-dependent effective mass m and the self-energy shift Δ are obtained either from microscopic calculations or, as proposed here, from the sum rules. Through the paper we will understand now the masses as effective masses.

From microscopic approaches, the effective self-energy shift and the effective mass are derived from the real part of the self-energy $\sigma(p, \omega)$, which determines the quasiparticle energy ϵ via

$$\epsilon = \frac{p^2}{2m_0} + \sigma(p, \epsilon). \quad (16)$$

The velocity of the quasiparticles is given by $\partial\epsilon/\partial p$, which leads to the definition of the effective mass

$$\frac{1}{m} = \frac{\frac{1}{m_0} + \frac{1}{p} \partial_p \sigma}{1 - \partial_\omega \sigma} \Bigg|_{\omega = \epsilon_f, p = p_f}, \quad (17)$$

where the momenta and energy are set to the Fermi momenta and energy after derivatives. Consequently the quasiparticle energy can be approximated by $\epsilon \approx p^2/2m + \Delta$ with the effective mass (17) and the energy shift $\Delta = \sigma(p_f, \epsilon_f) + p_f^2/2(1/m_0 - 1/m)$. This approximation has to be replaced by thermal averaging when finite temperature systems are considered. A useful method would also be to read off the quasiparticle parametrization from current parametrizations of the momentum distribution.^{43,44}

Using the definition of the compressibility one obtains directly from Eq. (15)

$$\begin{aligned} \mathcal{K} &= \frac{1}{n^2} \frac{\partial n}{\partial \mu} = -\frac{\beta}{n^2} \int \frac{dp}{(2\pi)^3} F(p)[1 - F(p)] \\ &\quad \times \left(\left[\frac{\partial \Delta(n)}{\partial n} - \frac{p^2}{2m} \frac{\partial \ln m}{\partial n} \right] \frac{\partial n}{\partial \mu} - 1 \right) \\ &= \frac{\mathcal{K}_0}{1 + n^2 \frac{\partial \Delta}{\partial n} \mathcal{K}_0 - \frac{3}{2} \frac{\partial \ln m}{\partial n}}, \end{aligned} \quad (18)$$

where the free compressibility is $\mathcal{K}_0 = (\beta/n^2) \int [dp/(2\pi)^3] F(p)[1 - F(p)]$. Alternatively, the energy shift Δ and the effective mass can be expressed by the Landau parameter.

In the following section we will present a consistent dynamical response function for the quasiparticle picture such that the correlations are parametrized by quasiparticles with an effective mass, an energy shift, and a relaxation time. From this we will obtain the correct compressibility (18) from the dynamical response via the static limit obeying the frequency sum rules. Actually, a static local field can be constructed provided we choose the effective mass appropriately. This will lead to a method for determining the effective mass from the structure factor, which is well known from Monte Carlo simulations or experiments.

The conventional compressibility sum rule⁴⁵ reads, using $\lim_{q \rightarrow 0} \Pi(0, q) = -n^2 \mathcal{K}_0$ and Eq. (6),

$$\begin{aligned}
-\lim_{q \rightarrow 0} \frac{2}{\pi V_q} \int_0^\infty \frac{d\omega'}{\omega'} \text{Im } \epsilon(\omega') &= \lim_{q \rightarrow 0} \text{Re} \frac{\Pi(0, q)}{1 - f_q(0) \Pi(0, q)} \\
&= -\lim_{q \rightarrow 0} \frac{n^2 \mathcal{K}_0}{1 + f_q(0) n^2 \mathcal{K}_0} \\
&\equiv -n^2 \mathcal{K}, \tag{19}
\end{aligned}$$

such that we can expect from the correct result (18) that the static local field has the form

$$\lim_{q \rightarrow 0} f_q(0) = \frac{\partial \Delta}{\partial n} - \frac{3}{2n^2 \mathcal{K}_0} \frac{\partial \ln m}{\partial \ln n}. \tag{20}$$

We will present a dynamical local field which leads in the static limit exactly to this desired result (20).

B. Frequency sum rules

The sum rules can be easily read off from the fact that the response function is an analytical function in the upper half plane and falls off with large frequencies faster than $1/\omega^2$ such that the compact Kramers-Kronig relation reads

$$\int d\omega' \frac{\chi(\omega')}{\omega' - \omega + i0} = 0 \tag{21}$$

closing the contour of integration in the upper half plane. From this, one has

$$\text{Re } \chi(\omega) = \int \frac{d\omega'}{\pi} \frac{\text{Im } \chi(\omega')}{\omega' - \omega} = \frac{\langle \omega \rangle}{\omega^2} + \frac{\langle \omega^3 \rangle}{\omega^4} + \dots \tag{22}$$

with the moments

$$\langle \omega^{2k+1} \rangle = \int \frac{d\omega}{\pi} \omega^{2k+1} \text{Im } \chi(\omega). \tag{23}$$

The first two moments are known exactly to be (Appendix C)

$$\langle \omega \rangle = \int \frac{d\omega}{\pi} \omega \text{Im } \chi(\omega) = \frac{nq^2}{m} \tag{24}$$

with the density n and mass m of the particles and^{1,7,8}

$$\langle \omega^3 \rangle = \int \frac{d\omega}{\pi} \omega^3 \text{Im } \chi(\omega) = 2E_{int} \frac{q^4}{m^2} + \frac{nq^6}{4m^3} - \frac{n^2 q^4}{m^2} V_q \tilde{I}(q). \tag{25}$$

Here E_{int} is the kinetic energy of the interacting system and

$$\begin{aligned}
\tilde{I}(q) &= -\frac{1}{n} \int \frac{dk}{(2\pi)^3} (S_{k-q} - S_k + n \delta_{k,q} - n \delta_{k,0}) \frac{(kq)^2}{q^4} \frac{V_k}{V_q} \\
&= I(q) - 1, \tag{26}
\end{aligned}$$

where $I(q)$ is usually presented in the literature,^{1,7}

$$I(q) = -\frac{1}{n} \int \frac{dk}{(2\pi)^3} (S_{k-q} - S_k) \frac{(kq)^2}{q^4} \frac{V_k}{V_q}, \tag{27}$$

and S_k is the structure factor (10).

In order to understand the different contributions, the short-distance limit (C26) from Eq. (26) is performed,

$$\begin{aligned}
\lim_{q \rightarrow \infty} \tilde{I}(q) &= -\frac{1}{n} \int \frac{dk}{(2\pi)^3} (S_k - 1 + n \delta_{k,0}) \\
&\quad \times \left[\frac{[(k+q)q]^2}{q^4} \frac{V_{k+q}}{V_q} - \frac{(kq)^2}{q^4} \frac{V_k}{V_q} \right] \\
&= (1 - g_0) + \lim_{q \rightarrow \infty} \frac{1}{n} \int \frac{dk}{(2\pi)^3} (S_k - 1) \frac{(kq)^2}{q^4} \frac{V_k}{V_q} - 1, \tag{28}
\end{aligned}$$

where the last term comes from the $\delta_{k,0}$ term. The first term alone is sometimes called the exact result,^{1,4,5,10} which holds only for static local fields. The second term describes the motion of particles inside the correlation hole, and becomes for the Coulomb case just $-\frac{1}{3}(1 - g_0)$, which has been pointed out in Ref. 9. Together, one obtains the small-distance result

$$\lim_{q \rightarrow \infty} \tilde{I}(q) = \frac{2}{3}(1 - g_0) - 1, \tag{29}$$

in agreement with the direct expansion (C26).

Now we proceed and derive the boundaries for the local field $f_q(\omega)$ from Eq. (4) using the above sum rules. Therefore we look at the large- ω expansion of Eq. (4) from which we can check with the help of Eq. (22) the desired sum rules (24) and (25). The simple RPA leads to [see also Eqs. (47)–(50)]

$$\Pi_0(\omega) = \frac{nq^2}{m\omega^2} + \left(2E \frac{q^4}{m^2} + \frac{nq^6}{4m^3} \right) \frac{1}{\omega^4} + o(1/\omega^5), \tag{30}$$

from which one gets with Eq. (4)

$$\begin{aligned}
\chi(\omega) &= \frac{nq^2}{m\omega^2} + \left(2E \frac{q^4}{m^2} + \frac{nq^6}{4m^3} + \frac{n^2 q^4}{m^2} [V_q + f_q(\infty)] \right) \frac{1}{\omega^4} \\
&\quad + o(1/\omega^5). \tag{31}
\end{aligned}$$

The first-order energy weighted sum rule (24) is fulfilled trivially, provided Π fulfills it. The third-order sum rule (25) can be fulfilled if we construct the local field according to Ref. 1,

$$\begin{aligned}
f_q(\infty) &= -V_q [1 + \tilde{I}(q)] - \frac{2}{n^2} (E - E_{int}) \\
&= -V_q I(q) - \frac{2}{n^2} (E - E_{int}), \tag{32}
\end{aligned}$$

where E is the kinetic energy of the noninteracting system. The last term describes the fact that the third-order frequency sum rule of the polarization function yields the noninteracting kinetic energy. This form, neglecting the last term, has been discussed in Ref. 7. In the later derivation of the polarization function we cannot consider the kinetic energy as

being interaction-free anymore, since the relaxation time appears as well as the effective mass. Therefore within the quasiparticle picture used here the difference $E - E_{int}$ vanishes or, positively stated, is accounted for by the effective mass. To facilitate the comparison with the literature we have kept this difference formal as $\Delta E = -(2/n^2)(E - E_{int})$.

With Eq. (32) we have given the constraint on the dynamical local field from the third-order frequency sum rule. In the following we will present a dynamical local field which fulfills both requirements, the compressibility (20) and the frequency sum rule (32).

III. DYNAMICAL RESPONSE FUNCTION

In Refs. 42 and 46 was given the polarization function for an interacting quantum system, imposing conservation laws on the relaxation-time approximation. These polarization functions we have denoted by Π^n for density conservation imposed, $\Pi^{n,j}$ for density and current conservation, and $\Pi^{n,j,E}$ for density, current, and energy conservation. In the former paper we could give only formal matrix expressions for the response function. In Appendix A we repeat briefly the derivation from the quantum kinetic theory and give now the explicit form of the response function. We obtain with Eqs. (A15) and (A16)

$$\chi(\omega) = \frac{\Pi^{n,j,E}(\omega)}{1 - V_0 \Pi^{n,j,E}(\omega) - 2mV_4 \Pi_{13}(\omega)}, \quad (33)$$

where

$$\Pi_{13}(\omega) = \frac{\Pi^{n,j,E} \Pi_h \Pi_2(0) - i\tau\omega \Pi_2\left(\omega + \frac{i}{\tau}\right)}{2m \frac{\Pi_h \Pi_0(0) - i\tau\omega \Pi_0\left(\omega + \frac{i}{\tau}\right)}{\Pi_h^2\left(\omega + \frac{i}{\tau}\right) - \Pi_0\left(\omega + \frac{i}{\tau}\right) \Pi_4\left(\omega + \frac{i}{\tau}\right)}}, \quad (34)$$

and

$$V_0 = \frac{\partial \Delta}{\partial n} - V_4 \frac{q^2}{4} + V_q, \quad (35)$$

$$V_4 = \frac{\partial}{\partial n} \frac{1}{2m} = -\frac{1}{2nm} \frac{\partial \ln m}{\partial \ln n}.$$

The explicit expressions of the moments of the polarization function are summarized in Appendix B for computation. From the response function (33) we will read off the main result of this paper: the dynamical local field for quasiparticles with the effective mass and energy. Now we are going to work out explicitly the form of the local field to show that the third-order sum rule can be fulfilled and the correct compressibility is obtained.

A. Dynamical local field

Comparing Eq. (33) with Eq. (4), an intermediate dynamical local field can be read off as $[V_0 = (\partial/\partial n)\Delta - V_4 q^2/4 + V_q]$

$$\begin{aligned} \tilde{f}_q(\omega) &= \frac{\partial \Delta}{\partial n} + V_4 \left(\frac{\Pi_h \Pi_2(0) - i\tau\omega \Pi_2\left(\omega + \frac{i}{\tau}\right)}{\Pi_h \Pi_0(0) - i\tau\omega \Pi_0\left(\omega + \frac{i}{\tau}\right)} - \frac{q^2}{4} \right) \\ &= \frac{\partial \Delta}{\partial n} + V_4 \left(\frac{\Pi_2(0)}{\Pi_0(0)} - \frac{q^2}{4} \right) + o\left(\frac{1}{\omega}\right) \\ &= \frac{\partial \Delta}{\partial n} - \frac{\partial \ln m}{\partial \ln n} \left\{ \frac{3}{2n^2 K_0} + o(q^2) \right. \\ &\quad \left. \frac{1}{3} \frac{E}{n^2} + o(1/q^2) + o\left(\frac{1}{\omega}\right) \right\}, \end{aligned} \quad (36)$$

where we used the expansion of Appendix B, explicitly Eq. (B16), in the first line and Eqs. (B14) and (B15) in the last line. Please note that $\Pi^{n,j,E}$ itself contains correlations beyond the polarization in RPA, Π_0 . This we will present in a moment.

First, we see the astonishing result that obviously

$$\lim_{\omega \rightarrow 0} \tilde{f}_q(\omega) = \lim_{\omega \rightarrow \infty} \tilde{f}_q(\omega), \quad (37)$$

the static local field required for the compressibility agrees with the infinite-frequency limit required for the third-order sum rule (31). [One should not be misled to the conclusion that this violates the Kramers-Kronig relation for $\tilde{f}_q(\omega)$. A toy example of $\text{Im} \tilde{f} = \sin(a\omega)/(\omega^2 - 4\pi^2/a^2)$ and the corresponding real part obtained from the Kramers-Kronig relation (22) shows that indeed Eq. (37) can hold simultaneously with the Kramers-Kronig relation.] This shows that the answer to the sum-rule puzzle is not due to the explicit dynamical character of the local field as often claimed in the literature. Instead we will see in Sec. III D that it is due to the underlying self-energy correction which has to obey certain relations.

At this point it is important to avoid a misunderstanding. The intermediate dynamical local field \tilde{f}_q is not the total one describing correlations beyond the RPA polarization function Π_0 , which would be the case only in the infinite-frequency limit. Instead, part of the correlations are already captured in $\Pi^{n,j,E}$. To make this explicit we write Eq. (33) as

$$\begin{aligned} \frac{1}{\chi(\omega)} &= \frac{1}{\Pi^{n,j,E}(\omega)} - V_q - \tilde{f}_q(\omega) \\ &= \frac{1}{\Pi_0(\omega)} - V_q - \tilde{f}_q(\omega) + \tilde{f}_q^*(\omega), \end{aligned} \quad (38)$$

where the difference between $\Pi^{n,j,E}$ and Π_0 has been recast into a local-field contribution⁴⁶ derived from Eq. (A12)–(A14),

$$\begin{aligned}
\tilde{f}_q^*(\omega) &= \frac{1}{\Pi^{\text{n,j,E}}(\omega)} - \frac{1}{\Pi_0(\omega)} \\
&= -\frac{1}{1-i\omega\tau} \left(\frac{1}{\partial_\mu n} - \frac{2E}{n^2} \right) + o(q^2) \\
&= \frac{1}{1-i\omega\tau} \frac{8\epsilon_f}{15n} + o(q^4), \tag{39}
\end{aligned}$$

with the last line valid for zero temperature. On the contrary, in the static limit $\tilde{f}_q^*(0)=0$. Together with Eq. (36) we obtain an effective local field renormalizing the RPA,

$$\begin{aligned}
f_q^{\text{eff}}(\omega) &= \tilde{f}_q(\omega) - \tilde{f}_q^*(\omega) \\
&= \frac{\partial\Delta}{\partial n} - \frac{\partial \ln m}{\partial \ln n} \frac{3}{2n^2 K_0} + \frac{1}{1-i\omega\tau} \frac{2E}{n^2} + o(q^2) \\
&= \frac{\partial\Delta}{\partial n} - \frac{\epsilon_f}{n} \left(\frac{\partial \ln m}{\partial \ln n} + \frac{1}{1-i\omega\tau} \frac{8}{15} \right), \tag{40}
\end{aligned}$$

where the last line is again the zero-temperature limit. The high-frequency limit required for the third-order sum rule agrees with $f_q^{\text{eff}}(\infty) = \tilde{f}_q(\infty) = f_q(\infty)$.

B. Connection to density functionals

In order to establish the connection to the ground-state exact relations⁴⁷ of the exchange-correlation energy ϵ_{xc} , we see from Eq. (40)

$$\lim_{\omega \rightarrow 0} \lim_{q \rightarrow 0} f_q^{\text{eff}}(\omega) \equiv \frac{d^2}{dn^2} [n \epsilon_{\text{xc}}(n)] = \frac{\delta}{\delta n} \Delta - \frac{\epsilon_f}{n} \left(\frac{\partial \ln m}{\partial \ln n} + \frac{8}{15} \right) \tag{41}$$

and

$$\lim_{q \rightarrow 0} f_q^{\text{eff}}(\infty) \equiv -\frac{4}{5} n^{2/3} \frac{d}{dn} \left[\frac{\epsilon_{\text{xc}}(n)}{n^{2/3}} \right] = \frac{\delta}{\delta n} \Delta - \frac{\epsilon_f}{n} \frac{\partial \ln m}{\partial \ln n} \tag{42}$$

with $f_0^{\text{eff}}(0) < f_0^{\text{eff}}(\infty) < 0$. This establishes the link to time-dependent density-functional theories.⁴⁸⁻⁵⁰ An overview of different approximation schemes is given in Ref. 51. We will see in Sec. III D that in order to fulfill the third-order frequency sum rule we have to have an additional effective mass beyond ϵ_{xc} .

C. Compressibility sum rule

From Eq. (36) one sees immediately that the required form for the compressibility sum rule (20) appears, since $\Pi^{\text{n,j,E}}(0) = \Pi_0(0)$. Therefore we have derived a dynamical response function and a local field, which shows in the static limit the correct compressibility (18). This compressibility formula (18) can be checked alternatively by calculating explicitly the frequency integral in Eq. (19). The required small-wave-vector limit of the so-called screened structure function (19) takes the form ($\Pi = \Pi^{\text{n,j,E}}$)

$$\frac{n}{\beta} K = \lim_{q \rightarrow 0} \frac{1}{n\pi} \int \frac{d\omega}{1-e^{-\beta\omega}} \frac{\text{Im} \Pi(\omega) [1 - \tilde{f}_q(\omega) \text{Re} \Pi(\omega)] + \text{Im} \Pi(\omega) \tilde{f}_q(\omega) \text{Re} \Pi(\omega)}{[1 - \tilde{f}_q(\omega) \text{Re} \Pi(\omega)]^2 + [\tilde{f}_q(\omega) \text{Im} \Pi(\omega)]^2}, \tag{43}$$

where $\tilde{f}_q(\omega) = \bar{f}_q(\omega) - V_q$. Now we observe that

$$\begin{aligned}
\lim_{q \rightarrow 0} \text{Im} \Pi(\omega) &= \lim_{q \rightarrow 0} \text{Im} \Pi_0(\omega) \\
&= -\pi \int \frac{dp}{(2\pi)^3} (e^{-\beta\omega} - 1) \delta \left(\omega - \frac{pq}{m} \right) \\
&\quad \times F(p) [1 - F(p)] + o(q^2) \\
&= 0 + o(q^2) \tag{44}
\end{aligned}$$

vanishes for small q . Therefore we have to perform the limit in Eq. (43) in the distribution sense to obtain

$$\begin{aligned}
\frac{n}{\beta} K &= \lim_{q \rightarrow 0} \frac{1}{n\pi} \int \frac{d\omega}{1-e^{-\beta\omega}} \left(\frac{\text{Im} \Pi_0(\omega)}{1 - \tilde{f}_q \text{Re} \Pi(\omega)} \right. \\
&\quad \left. + \pi \text{Re} \Pi(\omega) \delta(1 - \tilde{f}_q \text{Re} \Pi(\omega)) \right). \tag{45}
\end{aligned}$$

It is not difficult to see that the second part vanishes and we obtain

$$\begin{aligned}
\frac{n}{\beta} K &= \frac{1}{n} \int \frac{dp}{(2\pi)^3} F(p) [1 - F(p)] \\
&\quad \frac{1}{1 - \tilde{f}_q \text{Re} \Pi(0)} \\
&= \frac{1}{n\beta} \frac{n^2 K_0}{1 + n^2 K_0 \frac{\partial\Delta}{\partial n} - \frac{3}{2} \frac{\partial \ln m}{\partial \ln n}}, \tag{46}
\end{aligned}$$

which agrees with Eq. (18).

Therefore, we have shown that the dynamical local field (36) from the response function (33) leads to the same compressibility (19). This gives, besides the compressibility sum rule already checked, a second proof that we have derived a dynamical local field which leads to the correct compressibility. The static limit will allow now to complete the compressibility and third-order frequency sum rule simultaneously.

D. Frequency sum rules

Now that we have the response function (33) at hand we can proceed and prove the frequency sum rules (24) and (25) explicitly. First we expand the polarization functions for large frequencies. The superscript denotes which conservation laws are obeyed, density (n), energy (E), and current (j). We obtain

$$\begin{aligned} \Pi^n(\omega) = & \frac{nq^2}{m\omega^2} - i \frac{nq^2}{m\omega^3\tau} + \left(2E \frac{q^4}{m^2} + \frac{nq^6}{4m^3} - \frac{nq^2}{m\tau^2} \right) \frac{1}{\omega^4} \\ & - i \frac{q^4}{m^2\omega^5\tau} \left(\frac{n^2}{\Pi_0(0)} + 6E - \frac{nm}{q^2\tau^2} + \frac{3nq^2}{4m} \right) + o\left(\frac{1}{\omega^6}\right), \end{aligned} \quad (47)$$

$$\Pi^{n,E}(\omega) = \Pi^n(\omega) + o\left(\frac{1}{\omega^5}\right), \quad (48)$$

$$\begin{aligned} \Pi^{n,j}(\omega) = & \frac{nq^2}{m\omega^2} + \left(2E \frac{q^4}{m^2} + \frac{nq^6}{4m^3} \right) \frac{1}{\omega^4} \\ & - i \frac{q^4}{m^2\omega^5\tau} \left(\frac{n^2}{\Pi_0(0)} + 2E + \frac{nq^2}{4m} \right) + o\left(\frac{1}{\omega^6}\right), \end{aligned} \quad (49)$$

$$\Pi^{n,j,E}(\omega) = \Pi^{n,j}(\omega) + o\left(\frac{1}{\omega^5}\right). \quad (50)$$

We see that the current conservation repairs some defiances of the Mermin-Das polarization function Π^n , which obeys only density conservation, in that the imaginary part shows a different frequency behavior,

$$\lim_{\omega \rightarrow \infty} \text{Im} \Pi^{n,j,E}(q, \omega) = \frac{n^2 q^4}{\omega^5 \tau m^2} \left(\frac{1}{\partial_\mu n} - \frac{2E}{n^2} \right), \quad (51)$$

$$\lim_{\omega \rightarrow \infty} \text{Im} \Pi^n(q, \omega) = - \frac{nq^2}{\omega^3 \tau m}. \quad (52)$$

The last formula corrects a misprint in formula (23) of Ref. 46. This different behavior of the imaginary part is also reflected in different expressions for the third-order moment [$o(1/\omega^4)$] or third-order sum rule.

From Eqs. (22) and (47)–(50) we read off the sum rules

$$\langle \omega \rangle = \int \frac{d\omega}{\pi} \omega \text{Im} \Pi(\omega) = \frac{nq^2}{m}, \quad (53)$$

which holds for each of Π^n , $\Pi^{n,j}$, $\Pi^{n,j,E}$, and χ . In contrast to that we will see now that the third-order sum rule gives different results for the inclusion of different conservations laws. Using the polarization function including density, energy, and momentum conservation we obtain from Eq. (49)

$$\langle \omega^3 \rangle = \int \frac{d\omega}{\pi} \omega^3 \text{Im} \Pi^{n,j,E}(\omega) = 2E \frac{q^4}{m^2} + \frac{nq^6}{4m^3}. \quad (54)$$

We remark that according to Eqs. (47)–(50), the Mermin-Das polarization (A14) including only density conservation or even additionally energy conservation (A13) would yield

to an additional $-nq^2/m\tau^2$ term, which is an artifact. This is repaired by additionally taking into account momentum conservation.

Comparing Eq. (25) with Eq. (54) we see that just the last terms are missing. In order to obtain this sum rule we have to use the response function (33) and not the polarization function for which this sum rule is actually designed. With Eqs. (36) and (31) one gets

$$\chi(\omega) = \Pi^{n,j,E}(\omega) + \frac{n^2 q^4}{m^2} \left(V_0 + \frac{\Pi_2(0)}{\Pi_0(0)} V_4 \right) \frac{1}{\omega^4} + o\left(\frac{1}{\omega^5}\right). \quad (55)$$

Consequently, the third-order sum rule (32) is rendered correctly if one sets

$$\begin{aligned} f_q(\infty) = & V_0 - V_q + V_4 \frac{\Pi_2(0)}{\Pi_0(0)} = \frac{\delta\Delta}{\delta n} + V_4 \left(\frac{\Pi_2(0)}{\Pi_0(0)} - \frac{q^2}{4} \right) \\ = & -V_q [1 + \tilde{I}(q)] + \Delta E. \end{aligned} \quad (56)$$

By the requirement (56) we have a possibility to fulfill the third-order sum rule exactly from the dynamical response as well as static local-field model.

E. Consequences on self-energies

Let us now work out what that means for our self-energy parametrization Δ and m . From Eq. (56) we obtain a determining condition for the effective mass and energy shift [$I(q) = 1 + \tilde{I}(q)$],

$$V_q I(q) = \frac{1}{2mn} \left(\frac{\Pi_2(0)}{\Pi_0(0)} - \frac{q^2}{4} \right) \frac{\partial \ln m}{\partial \ln n} - \frac{\partial \Delta}{\partial n} + \Delta E. \quad (57)$$

Since we work with the effective mass and shift parametrization of the quasiparticle energy, the difference between E and E_{int} , ΔE , vanishes but we keep it for completeness further on.

Applying the small-wave-vector limit (C25) and (36) we see now from Eq. (57) for Coulomb systems

$$\lim_{q \rightarrow 0} \left(\frac{\partial \Delta}{\partial n} - \frac{3}{2} \frac{1}{n^2 K_0} \frac{\partial \ln m}{\partial \ln n} \right) = \Delta E - \frac{2}{5} \frac{q^2 V_q}{k_f^2} \gamma + o(q^2). \quad (58)$$

Contrary to Eq. (57), the large-wave-vector or small-distance limit (C26) and (36) reads

$$\lim_{q \rightarrow \infty} \left(\frac{\partial \Delta}{\partial n} - \frac{1}{3} \frac{E}{n^2} \frac{\partial \ln m}{\partial \ln n} \right) = \Delta E - \frac{2}{3} (1 - g_0) V_q + o(1/q^2), \quad (59)$$

where the last term on the right side vanishes for Coulomb potentials and persists only for potentials whose range falls faster than Coulomb potentials.

If we assume homogeneous systems, where Δ and m become independent of the wave vector, Eqs. (58) and (59) determine the quasiparticle shift as well as the effective mass via

$$\frac{\partial \ln m}{\partial \ln n} = \frac{\frac{2q^2 V_q}{5k_f^2} \gamma}{\frac{3}{2} \frac{1}{n^2 K_0} - \frac{1}{3} \frac{E}{n^2}},$$

$$\frac{\partial \Delta}{\partial n} = \frac{\frac{2q^2 V_q}{5k_f^2} \gamma}{\frac{9}{2} \frac{1}{EK_0} - 1} + \Delta E - \frac{2}{3} (1 - g_0) V_q + o(1/q^2), \quad (60)$$

where the last term vanishes for Coulomb potentials. If we remember the relation between the self-energy σ and the effective mass (17) we can determine from Eq. (60) the thermal averaged self-energy and wave-function renormalization $\mathcal{Z} = (1 - \partial_\omega \sigma)^{-1}$. For the special case of zero temperature and neglecting the usually small $\partial_p \sigma$ part, it reads

$$\Delta = \frac{1}{10} q^2 V_q \int_0^n dn' \frac{\gamma(n')}{k_f^2(n')} + \int_0^n dn' \Delta E,$$

$$\ln \mathcal{Z}|_{\epsilon=\epsilon_f} = -m_0 q^2 V_q \int_0^n dn' \frac{\gamma(n')}{k_f^4(n')} \quad (61)$$

with γ from Eq. (9) such that the effective mass takes the form

$$m = m_0 \exp \left\{ m q^2 V_q \int_0^n dn' \frac{\gamma(n')}{k_f^4(n')} \right\}. \quad (62)$$

The general expression for finite temperatures is given by Eq. (60).

Since the needed expressions \tilde{I} in Eq. (26) or γ in Eq. (9) are functions of the structure function, which is given itself again by the response function (10), we have the usual self-consistent procedure analogous to Eq. (8) first introduced by STLS (Ref. 4) but with another $G(q)$. Here we suggest to obtain the effective mass m and energy shift from Eq. (57) using $I(q)$.

Alternatively one might use the well-known experimental values of the static structure factor S_q and determine this way the effective mass and energy shift. This definition of effective mass has the advantage that the third-order and compressibility sum rule of the response function will be rendered exactly. Therefore Eq. (60) is the second main result of this paper.

Let us remark that if we would have no effective mass but a mere density-dependent self-energy σ , such as in density-functional theories, the requirement of Eqs. (58) and (59) corresponding to the compressibility and third-order frequency sum rule cannot be fulfilled simultaneously. This was remarked in detail in literature.^{11,15} By including the effective mass, we can resolve this puzzle here.

IV. NUMERICAL RESULTS AND DISCUSSION

As a test example we will now consider the unpolarized electron gas in three dimensions (3D) at zero temperature.

TABLE I. The long-wavelength limit of the local-field factor γ_0 and the small-range value of the pair correlation according to the MC data of Ref. 23. The value in parentheses is an interpolation. The quasiparticle (QP), self-consistent quasiparticle (SQP), as well as Pathak-Vashishta value together with ΔE (PV+ ΔE) are given for comparison.

r_s	γ_0	δ	$1 - g(0)$			
	MC	MC	MC	SQP	QP	PV+ ΔE
1	0.2567	0.036	0.7276	0.7240	0.6626	0.6971
2		0.091	(0.8627)	0.8627	0.7666	0.8346
3	0.2722		0.9078	0.9201	0.8456	
5	0.2850	0.292	0.9768	0.9627	0.9351	1.0558
10	0.3079	0.619	0.9976	0.9733	0.9613	1.1231

The density parameter is the usual Bruckner parameter, defined as the ratio of the interparticle distance to the Bohr radius $r_s = (3/4\pi n)^{1/3}/a_0$. First we will give a simple quasiparticle picture (QP), where the Δ and effective mass are determined as density-dependent constants from Monte Carlo (MC) data. In the second step, we will allow that the Δ and the effective mass depend on the wave vector. This will lead to the self-consistent quasiparticle picture (SQP).

In order to calculate the quasiparticle parameter Δ and the effective mass, we employ the results of MC simulations.^{23,24} For a parametrization of the MC data see Ref. 52. In Ref. 1 was discussed the difference between interacting and free kinetic energies, $\Delta E = (2/n^2)(E_{int} - E)$. This difference is given as $\delta = E_{int}/E - 1$ by the MC data of Ceperley and Alder. In our quasiparticle picture one has $E_{int}/E = m_0/m$, and the effective mass is given by $m = m_0/(1 + \delta)$. This allows us to determine the needed derivative as

$$\frac{\partial \ln m}{\partial \ln n} = \frac{r_s}{3(1 + \delta)} \frac{\partial \delta}{\partial r_s}. \quad (63)$$

The difference ΔE is given by the large-wavelength limit of the local field,

$$\lim_{q \rightarrow 0} G(q) = \gamma_0 \left(\frac{q}{k_f} \right)^2 = \lim_{q \rightarrow 0} \frac{1}{V_q} [V_q I(q) - \Delta E]$$

$$= \lim_{q \rightarrow 0} \frac{1}{V_q} \left(\frac{1}{2mn} \frac{\partial \ln m}{\partial \ln n} - \frac{\delta \Delta}{\delta n} \right), \quad (64)$$

which is presented by γ_0 ,²³ see Table I. This allows us to determine the quasiparticle energy $\delta \Delta / \delta n$, since the last line of Eq. (64) is just Eq. (57). The first model can be called the improved Pathak/Vashishta scheme (PV+ ΔE) while the second one together with the effective mass (63) establishes the quasiparticle picture proposed here. We remark that, in order to realize a certain Bruckner parameter r_s , the quasiparticle picture must be calculated with $r_s(1 + \delta)$, since all formulas work with the effective mass leading to $r_s/(1 + \delta)$.

With this determination of the QP parameters as well as (PV+ ΔE) from MC data we can now compare the results of the iteration scheme $f_q \rightarrow S_q \rightarrow I(q) \rightarrow f_q$. For zero temperature all formulas simplify and we give them here for convenience in dimensionless momentum $K=q/k_f$, energy $\Omega = \omega/\epsilon_f$, and distance $R=rk_f/\hbar$. Then the dimensionless effective local field is given by

$$f_K = - \left(\frac{2s^4}{9\pi^4} \right)^{1/3} r_s \left(\frac{I(K)}{K^2} + \gamma_0 - \frac{2}{5} \gamma \right) - \frac{r_s}{4(1+\delta)} \frac{\partial \delta}{\partial r_s} \left(1 - \frac{\Pi_2(0,K)}{\Pi_0(0,K)} + \frac{K^2}{4} \right) \quad (65)$$

with γ_0 from Eq. (64) and $\gamma = -1/s \int_0^\infty dK (S_K - 1)$ from Eq. (9) and the spin degeneracy for electrons $s=2$. The PV model would consist only of the term $I(K)$ on the right-hand side of Eq. (65) and the (PV+ ΔE) model takes into account the first line of Eq. (65). The QP finally takes all terms into account where we have used Eq. (56) or (57) and the requirement (64). The dimensionless function $\Pi_2(0,K)/\Pi_0(0,K) = \Pi_2(0)/k_f^2 \Pi_0(0)$ plotted in Fig. 5 is given by

$$\frac{\Pi_2(0,K)}{\Pi_0(0,K)} = \frac{1}{2} \frac{3 - \frac{K^2}{4} - \frac{1}{4K} \left(1 - \frac{K^2}{4} \right)^2 \ln \left| \frac{2-K}{2+K} \right|}{1 - \frac{1}{4K} \left(1 - \frac{K^2}{4} \right) \ln \left| \frac{2-K}{2+K} \right|} = \frac{1}{4} \begin{cases} 1 - \frac{K^2}{3} + o(K^4) \\ \frac{K^2}{4} + \frac{1}{5} - \frac{48}{175K^2} + o(K^{-4}). \end{cases} \quad (66)$$

Provided we know the effective local field, f_K in Eq. (65), the static structure factor can be obtained from Eq. (10) as

$$S_K = \frac{3}{4\pi} \int_0^\infty d\Omega \operatorname{Im} \frac{\Pi_0(\Omega, K)}{1 - \left[f_K + \left(\frac{2s^4}{9\pi^4} \right)^{1/3} \frac{r_s}{K^2} \right] \Pi_0(\Omega, K)}, \quad (67)$$

where we have used the zero-temperature dimensionless quantum polarization from Eq. (B1),

$$\Pi_0(\Omega, K) = -1 + \frac{4K^2 - (\Omega - K^2)^2}{8K^3} \ln \frac{2K + \Omega - K^2}{2K - \Omega + K^2} - \frac{4K^2 - (\Omega + K^2)^2}{8K^3} \ln \frac{2K + \Omega + K^2}{2K - \Omega - K^2} + i \frac{\pi}{2} \times \begin{cases} 0 \\ \frac{\Omega}{K} & \text{for } K < 2 \text{ and } |\Omega| < |K^2 - 2K| \\ \frac{4K^2 - (\Omega - K^2)^2}{4K^3} & \text{for } |K^2 - 2K| < |\Omega| < |K^2 + 2K|. \end{cases} \quad (68)$$

With the help of the static structure factor we have the pair-correlation function (11),

$$g_R = 1 + \frac{3}{sR} \int_0^\infty dK K \sin(KR) (S_K - 1), \quad (69)$$

from which the required $I(K)$ function reads according to Eq. (C24)

$$I(K) = -2 \int_0^\infty \frac{dR}{R} (g_R - 1) j_2(KR) \quad (70)$$

with the spherical Bessel function $j_2(x)$. This function now enters Eq. (65), closing the iteration.

In Table I we compare the small-distance value of the pair correlation (11) of the PV+ ΔE model with the QP model. We see that for more dense systems the PV+ ΔE model leads to correlations that are too large, while the QP model gives values lower than the MC values at higher r_s . In Fig. 1 we compare the static structure factor of the two models with the MC data. We see that a difference occurs between the PV+ ΔE and QP model at higher r_s .

The difference between the models becomes more apparent if we plot the local-field factor as in Figs. 2–4. We see that the simple PV model underestimates the MC data, though it satisfies the third-order frequency sum rule. This result is improved by adding the ΔE , read off from the large-wavelength limit of MC data. Further improvement is achieved in the QP. At smaller densities, $r_s=2$, the local field is overestimated at higher wave vectors, which leads to the deviation seen in Table I.

The QP curves show a small hump at $q=2k_f$ in contrast to the PV+ ΔE model. This comes from the function $\Pi_2(0)/\Pi_0(0)$, which is plotted in Fig. 5.

While in 3D this hump at $q=2k_f$ is not much pronounced, it shows up in 2D systems.⁵³ With the help of the formulas in Appendix B one can present also the 2D results, which should be devoted to another paper.

According to Eq. (57) the functional form of Π_2/Π_0 on the right-hand side should be equal to $I(k)$ which is a smooth function according to Figs. 2–4. Therefore with the simple quasiparticle picture considered so far one cannot satisfy the third-order sum rule for all q . In order to achieve this, we must allow Δ as well as the effective mass to have a q

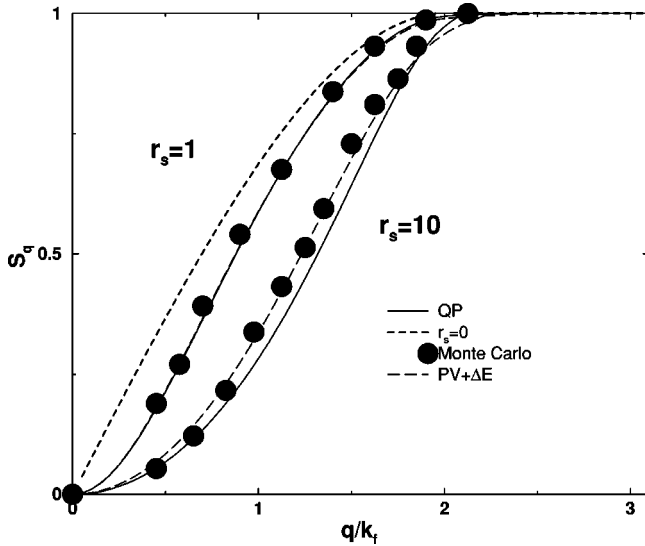


FIG. 1. The static structure factor for $r_s=0$, $r_s=1$ and $r_s=10$ from the PV, the PV + ΔE , and QP model compared to the MC data (Ref. 23) as presented in Ref. 25.

dependence. Of course this leads to a self-consistent quasiparticle picture, since the energies under integration of the polarization function now change their dispersion. The iteration scheme is therefore enlarged to $f_q \rightarrow S_q \rightarrow I(q) \rightarrow \Delta(q), m(q) \rightarrow f_q$ according to Eq. (57). We call this iteration here SQP. It satisfies the third-order frequency sum rule and the compressibility sum rule simultaneously for all q . The results describe the MC data in Figs. 2–4. Also, the small-distance value of the pair-correlation function is now in better agreement with the MC data as can be seen in Table I.

V. SUMMARY

We have derived a response function in the quasiparticle picture where the correlations are parametrized by a density-

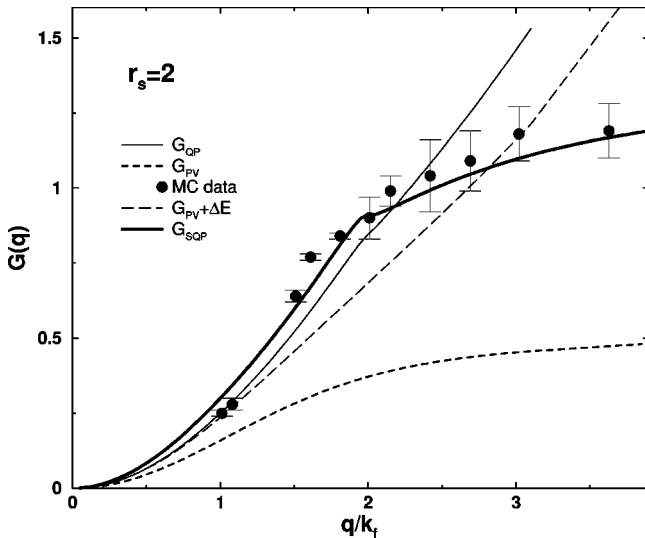


FIG. 2. The static local field for $r_s=2$ from the PV, the PV + ΔE , and QP model compared to the MC data (Ref. 24).

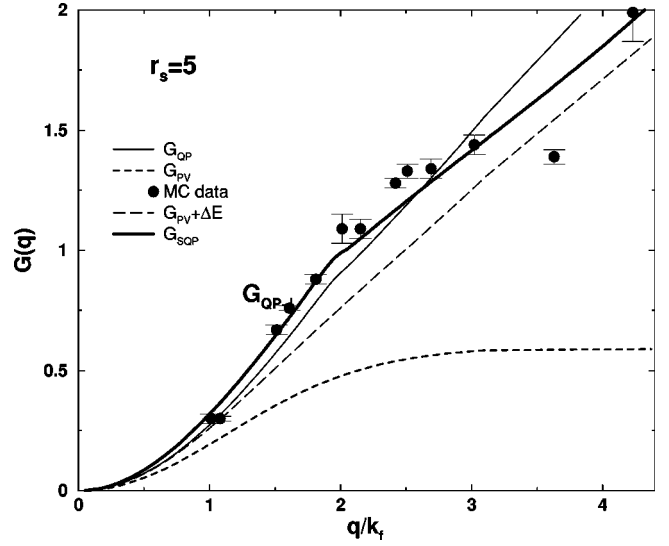


FIG. 3. The static local field for $r_s=5$ from the PV, the PV + ΔE , and QP model compared to the MC data (Ref. 24).

dependent effective mass, energy shift, and a relaxation time respecting density, energy, and momentum conservation. The dynamical response function can be given in the form of a modified RPA including a dynamical local field. This local field leads in the static limit to the correct compressibility. The effective mass and quasiparticle energy shift are proposed to be determined by the requirement of the third-order sum rule. This allows in turn to satisfy the compressibility sum rule simultaneously. Since the effective mass is now a function of the structure factor, one might use experimentally known values or simulation results to construct a more realistic quasiparticle picture. The consequences on microscopic expressions of the self-energy are presented. The thermal averaged self-energy and wave-function renormalization, i.e., the frequency derivative of the self-energy, are linked to the pair-correlation function at small distances.

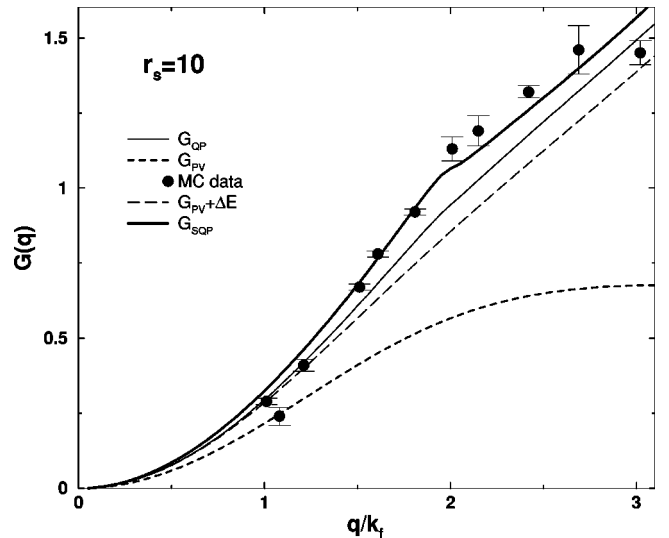


FIG. 4. The static local field for $r_s=10$ from the PV, the PV + ΔE , and QP model compared to the MC data (Ref. 24).

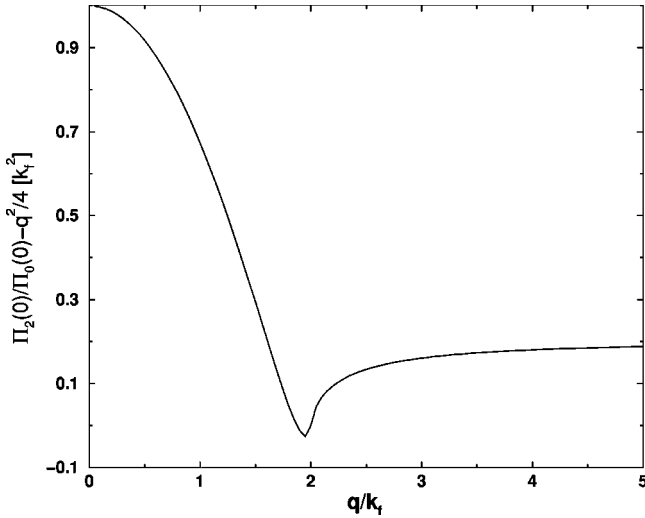


FIG. 5. $\Pi_2(0)/\Pi_0(0) - q^2/4$ of Eq. (57) or explicitly Eq. (66) for three dimensions at zero temperature.

While all the expressions we derived are valid for finite temperatures, we have compared them as a test example with the Monte Carlo data for an electron gas at zero temperature. We find an improved description by the Pathak-Vashishta scheme accomplished by an energy shift derived from MC data. The best agreement with the data is achieved by constructing a nonlocal quasiparticle picture allowing for a wave-vector-dependent effective mass and an energy shift in the form of a self-consistent quasiparticle picture.

ACKNOWLEDGMENTS

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APPENDIX A: DYNAMIC RESPONSE FUNCTION

In a former paper,^{42,46} the density, current, and energy response $\{\chi, \chi_J, \chi_E\} = \mathcal{X}\{1, 0, 0\}^T$ of an interacting quantum system

$$\begin{pmatrix} \delta n \\ q \cdot \delta J \\ \delta E \end{pmatrix} = \begin{pmatrix} \chi \\ \chi_J \\ \chi_E \end{pmatrix} V^{\text{ext}} \equiv \mathcal{X} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} V^{\text{ext}} \quad (\text{A1})$$

to the external perturbation V^{ext} were derived formally, provided the density, momentum, and energy are conserved. This has been achieved by linearizing the kinetic equation for the one-particle density operator $\hat{\rho}$ in the relaxation-time approximation

$$\hat{\rho} + i[\hat{\mathcal{E}} + \hat{V}^{\text{ext}}, \hat{\rho}] = \frac{\hat{\rho}^{\text{le.}} - \hat{\rho}}{\tau}, \quad (\text{A2})$$

where the relaxation was considered with respect to the local-density operator $\hat{\rho}^{\text{le.}}$ or the corresponding local equilibrium distribution function

$$F(p) = \left[\left(\frac{\varepsilon_0[p - Q(R, t)] - \mu(R, t)}{T(R, t)} \right) + 1 \right]^{-1}. \quad (\text{A3})$$

This local equilibrium is given by a local time-dependent chemical potential μ , a local temperature T , and a local mass motion momentum Q . These local quantities have been specified by the requirement that the expectation values for density, momentum, and energy are the same as the expectation values performed with F , which ensures conservation laws.

The correlations are shared in the kinetic equation (A2) in such a way that the energy operator $\hat{\mathcal{E}}$ parametrizes the density-dependent quasiparticle energy or variation of the energy functional in the Landau liquid (momentum dependent) or density-functional sense (momentum independent), and the collision integral is approximated by a conserving relaxation-time approximation. While in Ref. 42 the general density-, energy-, and momentum-dependent form of such a parametrization has been discussed we want to consider now only a special case of an effective-mass and rigid shift parametrization,

$$\hat{\mathcal{E}} = -\nabla \left(\frac{1}{2m(\hat{n})} \right) \nabla + \Delta(\hat{n}), \quad (\text{A4})$$

such that the variation $\mathcal{E}(n) = \mathcal{E}_0 + \delta\mathcal{E}$ reads $[p = (p_1 + p_2)/2, q = p_1 - p_2]$

$$\delta\mathcal{E} = \langle p_1 | \delta\hat{\mathcal{E}} | p_2 \rangle = (V_0 + V_4 p^2) \delta n(q) \quad (\text{A5})$$

with

$$V_0 = \frac{\partial}{\partial n} \Delta - V_4 \frac{q^2}{4} + V_q, \quad (\text{A6})$$

$$V_4 = \frac{\partial}{\partial n} \frac{1}{2m} = -\frac{1}{2nm} \frac{\partial \ln m}{\partial \ln n}.$$

The response matrix (A1) can be given in terms of the polarization matrix \mathcal{P} , see Eq. (29) of Ref. 42, which is the response of the kinetic equation without the self-consistent quasiparticle energies $\delta\mathcal{E}$. The response reads

$$\mathcal{X} = (\mathcal{I} - \mathcal{P}\mathcal{G}^{-1}\mathcal{V})^{-1}\mathcal{P} \quad (\text{A7})$$

with the matrices simplified for our considered case (A5),

$$\mathcal{V} = \begin{pmatrix} g_1 V_0 + g_{p^2} V_4 & 0 & 0 \\ g_{pq} V_0 + g_{p^2 pq} V_4 & 0 & 0 \\ g_\epsilon V_0 + g_{p^2 \epsilon} V_4 & 0 & 0 \end{pmatrix}_{\omega+i\tau}, \quad (\text{A8})$$

$$\mathcal{G} = \begin{pmatrix} g_1 & g_{pq} & g_\epsilon \\ g_{pq} & g_{(pq)^2} & g_{pq\epsilon} \\ g_\epsilon & g_{\epsilon pq} & g_{\epsilon\epsilon} \end{pmatrix}_{\omega+i\tau}, \quad (\text{A9})$$

and the correlation functions $[\varepsilon = p^2/2m + \Delta]$ are defined as

$$g_\phi(\omega) = \int \frac{dp}{(2\pi)^3} \phi \frac{F\left(p + \frac{q}{2}\right) - F\left(p - \frac{q}{2}\right)}{\varepsilon\left(p + \frac{q}{2}\right) - \varepsilon\left(p - \frac{q}{2}\right) - \omega - i0}. \quad (\text{A10})$$

Explicit formulas are in Appendix B. We keep the matrix notation of Ref. 42 also for this special case in order to convince the reader about the technical usefulness of such notation. The 3×3 polarization matrix $\mathcal{P} = \{\Pi_{nm}\}$ contains the corresponding density, momentum, and energy polarizations as

$$\begin{pmatrix} \delta n \\ \delta q J \\ \delta E \end{pmatrix} = \begin{pmatrix} \Pi_{11} \\ \Pi_{21} \\ \Pi_{31} \end{pmatrix} V^{\text{ind}}. \quad (\text{A11})$$

In fact as found in Ref. 46 it is possible to express the density polarization function $\Pi_{11} \equiv \Pi^{\text{n,j,E}}$, including density, current, and energy conservation, by a simpler one containing density and energy conservation $\Pi^{\text{n,E}}$ as

$$\frac{1}{\Pi^{\text{n,j,E}}(\omega)} - \frac{1}{\Pi^{\text{n,E}}(\omega)} = \frac{1}{\Pi^{\text{n,j}}(\omega)} - \frac{1}{\Pi^{\text{n}}(\omega)} = -\frac{i\omega}{\tau} \frac{m}{nq^2}. \quad (\text{A12})$$

This shows that the momentum conservation leads simply to a dynamical local-field correction. The energy- and density-conserving polarization function reads explicitly

$$\Pi^{\text{n,E}}(\omega) = (1 - i\omega\tau) \left(\frac{g_1\left(\omega + \frac{i}{\tau}\right)g_1(0)}{h_1} - \omega\tau i \frac{[h_\varepsilon g_1(0) - h_1 g_\varepsilon(0)]^2}{h_1(h_\varepsilon^2 - h_\varepsilon h_1)} \right), \quad (\text{A13})$$

where we use the abbreviation $h_\phi = g_\phi(\omega + i/\tau) - \omega\tau i g_\phi(0)$. The first part is just the known Mermin-Das polarization function including only density conservation,^{54,55}

$$\begin{aligned} \Pi^{\text{n}}(\omega) &= \frac{\Pi_0(\omega + i/\tau)}{1 - \frac{1}{1 - i\omega\tau} \left[1 - \frac{\Pi_0(\omega + i/\tau)}{\Pi_0(0)} \right]} \\ &= (1 - i\omega\tau) \frac{g_1\left(\omega + \frac{i}{\tau}\right)g_1(0)}{h_1}. \end{aligned} \quad (\text{A14})$$

Now we want to give the full density response function $\chi = \mathcal{X}_{11}$ according to Eq. (A1). Due to the special considered case (A5) and consequently (A8), the density response function χ can be written from Eq. (A7) into ($\Pi_{11} = \Pi^{\text{n,j,E}}$)

$$\chi(\omega) = \frac{\Pi^{\text{n,j,E}}(\omega)}{1 - V_0 \Pi^{\text{n,j,E}}(\omega) - 2mV_4 \Pi_{13}(\omega)}, \quad (\text{A15})$$

where

$$\begin{aligned} \Pi_{13}(\omega) &= \frac{\Pi^{\text{n,j,E}} \Pi_h \Pi_2(0) - i\tau\omega \Pi_2\left(\omega + \frac{i}{\tau}\right)}{2m \frac{\Pi_h \Pi_0(0) - i\tau\omega \Pi_0\left(\omega + \frac{i}{\tau}\right)}{\tau}}, \\ \Pi_h &= \frac{\Pi_2^2\left(\omega + \frac{i}{\tau}\right) - \Pi_0\left(\omega + \frac{i}{\tau}\right) \Pi_4\left(\omega + \frac{i}{\tau}\right)}{\Pi_2^2(0) - \Pi_0(0) \Pi_4(0)} \end{aligned} \quad (\text{A16})$$

are expressed in terms of moments of the correlation function (B1). The response function (33) is the main result of this paper since it gives the consistent response function for the quasiparticle consisting of effective mass, energy, and relaxation time.

APPENDIX B: EXPLICIT FORMULAS OF CORRELATION FUNCTIONS

The different occurring correlation functions (A10) can be written in terms of moments of the usual Lindhard polarization function Π_0 ,

$$\Pi_n = s \int \frac{dp}{(2\pi)^D} p^n \frac{F\left(p + \frac{q}{2}\right) - F\left(p - \frac{q}{2}\right)}{\frac{pq}{m} - \omega - i0} \quad (\text{B1})$$

as

$$\begin{aligned} g_1 &= \Pi_0, \\ g_{pq} &= m\omega \Pi_0, \\ g_\varepsilon &= \frac{\Pi_2}{2m}, \\ g_{\varepsilon p^2} &= \frac{\Pi_4}{2m}, \\ g_{p^2 pq} &= m\omega \Pi_2, \\ g_{(pq)^2} &= -mq^2 n + m^2 \omega^2 \Pi_0. \end{aligned} \quad (\text{B2})$$

Here s is the spin degeneracy and D gives the dimension of the system. While all formulas in the text are written for the three-dimensional case, they hold equally for one and two dimensions.

For practical and numerical calculations we can rewrite the Π_n by polynomial division as

$$\Pi_2 = -mn + \frac{m^2 \omega^2}{q^2} \Pi_0 + \tilde{\Pi}_2,$$

$$\begin{aligned} \Pi_4 = & -\frac{nmq^2}{4} \left(1 + \frac{4m^2\omega^2}{q^4} \right) - \frac{m^4\omega^4}{q^4} \Pi_0 - \frac{2m^2\omega^2}{q^2} \tilde{\Pi}_2 \\ & - \tilde{\Pi}_4 - \frac{14}{3} m^2 E \times \begin{cases} 1 & \text{for } D=2,3 \\ \frac{1}{2} & \text{for } D=1, \end{cases} \end{aligned} \quad (\text{B3})$$

where the $\tilde{\Pi}_i$ are the projected moments perpendicular to \mathbf{q} and read

$$\begin{aligned} \tilde{\Pi}_2 = & s \int \frac{dp}{(2\pi)^D} \left(p - \frac{(pq)}{q^2} q \right)^2 \frac{F\left(p + \frac{q}{2}\right) - F\left(p - \frac{q}{2}\right)}{\frac{pq}{m} - \omega - i0} \\ = & m \int_{-\infty}^{\mu} d\mu' \Pi_0 \begin{cases} 2 & \text{for } D=3 \\ 1 & \text{for } D=1,2 \end{cases} \\ \approx & mT \Pi_0 \begin{cases} 2 & \text{for } D=3 \\ 1 & \text{for } D=1,2, \end{cases} \\ \tilde{\Pi}_4 = & s \int \frac{dp}{(2\pi)^D} \left(p - \frac{(pq)}{q^2} q \right)^4 \frac{F\left(p + \frac{q}{2}\right) - F\left(p - \frac{q}{2}\right)}{\frac{(pq)}{m} - \omega - i0} \\ = & m^2 \int_{-\infty}^{\mu} d\mu' \int_{-\infty}^{\mu'} d\mu'' \Pi_0 \begin{cases} 8 & \text{for } D=3 \\ 3 & \text{for } D=1,2 \end{cases} \\ \approx & m^2 T^2 \Pi_0 \begin{cases} 8 & \text{for } D=3 \\ 3 & \text{for } D=1,2. \end{cases} \end{aligned} \quad (\text{B4})$$

The corresponding last identities are valid only for nondegenerate, Maxwellian distributions with temperature T . The general form of the polarization functions is presented as an integral over the chemical potential μ of the Lindhard polarization Π_0 . This is applicable also to the degenerate case.

1. Long-wavelength expansion

In real situations it is often helpful to have the small-wave-vector expansion of the various occurring correlation functions. With the help of Eqs. (B4) and (B3) this can be tremendously simplified if the expansion for Π_0 is written as

$$\begin{aligned} \Pi_0(\omega) = & -\frac{s}{\omega} \int \frac{dp}{(2\pi)^D} \left(-\frac{(qp)^2}{m^2\omega} F' + \frac{q^2(qp)^2}{8m^3\omega} F'' \right. \\ & \left. - \frac{(qp)^4}{24m^4\omega} F''' - \frac{(pq)^4}{m^4\omega^3} F' \right) + o(q^5), \end{aligned} \quad (\text{B5})$$

where $F' = \partial_{\mu} F$, etc. For the static case we have

$$\Pi_0(0) = s \int \frac{dp}{(2\pi)^D} \left(-F' + \frac{q^2}{8m} F'' - \frac{(qp)^2}{24m^2} F''' \right) + o(q^4). \quad (\text{B6})$$

We give now the one-, two-, and three-dimensional cases separately.

a. 3D case

Since $\partial_p F = -p \partial_{\mu} F/m$, partial integration gives

$$\int \frac{dp}{(2\pi)^3} F' G(p) = m \int \frac{dp}{(2\pi)^3} \frac{F}{p^2} \partial_p [pG(p)] \quad (\text{B7})$$

and applied to Eq. (B5) one gets

$$\Pi_0(\omega) = \frac{q^2}{m\omega^2} n + \frac{2q^4}{m^2\omega^4} E + o(q^6). \quad (\text{B8})$$

The density n and energy E , and higher moments read in terms of

$$f_n = \frac{1}{\Gamma(n)} \int_0^{\infty} \frac{x^{n-1} dx}{e^{x-\beta\mu} + 1} \quad (\text{B9})$$

as

$$\begin{aligned} n = \langle 1 \rangle = & \frac{s}{\lambda^3} f_{3/2}, \\ E = \left\langle \frac{p^2}{2m} \right\rangle = & \frac{3}{2} \int^{\mu} d\mu' n = \frac{3}{2\beta} \frac{s}{\lambda^3} f_{5/2}, \\ E_2 = \left\langle \left(\frac{p^2}{2m} \right)^2 \right\rangle = & \frac{5}{2} \int^{\mu} d\mu' E = \frac{15}{4\beta^2} \frac{s}{\lambda^3} f_{7/2}, \\ E_3 = \left\langle \left(\frac{p^2}{2m} \right)^3 \right\rangle = & \frac{7}{2} \int^{\mu} d\mu' E_2 = \frac{105}{8\beta^3} \frac{s}{\lambda^3} f_{9/2}. \end{aligned} \quad (\text{B10})$$

With the help of Eqs. (B4) and (B3) one writes down immediately the higher-order correlation functions as

$$\begin{aligned} \tilde{\Pi}_2(\omega) = & \frac{4q^2}{3\omega^2} E + \frac{8q^4}{5m\omega^4} E_2, \\ \tilde{\Pi}_4(\omega) = & \frac{32mq^2}{15\omega^2} E_2 + \frac{64q^4}{35\omega^4} E_3. \end{aligned} \quad (\text{B11})$$

The static case (B6) yields with Eq. (B7),

$$\Pi_0(0) = -\partial_{\mu} n + \frac{q^2}{12m} \partial_{\mu}^2 n, \quad (\text{B12})$$

and with Eqs. (B3) and (B4)

$$\begin{aligned} \tilde{\Pi}_2(0) = & -2mn + \frac{q^2}{6} \partial_{\mu} n, \\ \tilde{\Pi}_4(0) = & -\frac{16}{3} m^2 E + \frac{2mq^2}{3} n. \end{aligned} \quad (\text{B13})$$

In the text we use also the small- and large-wave-vector limit of the static 3D polarization functions. Since

$$\Pi_0(0) = \begin{cases} -n^2 \mathcal{K}_0 + o(q^2) \\ -4n \frac{m}{q^2} - \frac{32m^2}{3q^4} E + o(1/q^6), \end{cases} \quad (\text{B14})$$

we obtain from Eqs. (B3) and (B4)

$$\Pi_2(0) = \begin{cases} -3mn + o(q^2) \\ -mn - \frac{16}{3} \frac{m^2}{q^2} E - \frac{128m^3}{15q^4} E_2 + o(1/q^6), \end{cases} \quad (\text{B15})$$

which leads to

$$\frac{\Pi_2(0)}{\Pi_0(0)} = \begin{cases} \frac{3m}{n\mathcal{K}_0 + o(q^2)} \\ \frac{q^2}{4} + \frac{2Em}{3n} + o(1/q^2). \end{cases} \quad (\text{B16})$$

b. 2D case

For two dimensions, we have instead of Eq. (B7),

$$\int \frac{dp}{(2\pi)^2} F' G(p) = m \int \frac{dp}{(2\pi)^2} F \partial_p G(p), \quad (\text{B17})$$

which applied to Eq. (B5) yields

$$\Pi_0(\omega) = \frac{2\pi q^2}{m\omega^2} n + \frac{6\pi q^4}{m^2\omega^4} E \quad (\text{B18})$$

and from Eqs. (B3) and (B4)

$$\begin{aligned} \tilde{\Pi}_2(\omega) &= \frac{2\pi q^2}{\omega^2} E + \frac{6\pi q^4}{m\omega^4} E_2, \\ \tilde{\Pi}_4(\omega) &= \frac{6\pi q^2 m}{\omega^2} E_2 + \frac{18\pi q^4}{\omega^4} E_3. \end{aligned} \quad (\text{B19})$$

The different occurring moments read here

$$\begin{aligned} n = \langle 1 \rangle &= \frac{s}{\pi\lambda^2} f_1, \\ E = \left\langle \frac{p^2}{2m} \right\rangle &= \int^\mu d\mu' n = \frac{1}{\beta} \frac{s}{\lambda^2} f_2, \\ E_2 = \left\langle \left(\frac{p^2}{2m} \right)^2 \right\rangle &= \int^\mu d\mu' E = \frac{1}{\beta^2} \frac{s}{\lambda^2} f_3, \\ E_3 = \left\langle \left(\frac{p^2}{2m} \right)^3 \right\rangle &= \int^\mu d\mu' E_2 = \frac{1}{\beta^3} \frac{s}{\lambda^2} f_4. \end{aligned} \quad (\text{B20})$$

The static case is now analogous and reads with Eq. (B17) from Eq. (B6)

$$\begin{aligned} \Pi_0(0) &= -\partial_\mu n + \frac{q^2}{24m} \partial_\mu^2 n, \\ \tilde{\Pi}_2(0) &= -mn + \frac{q^2}{24} \partial_\mu n, \\ \tilde{\Pi}_4(0) &= -3m^2 E + \frac{mq^2}{8} n. \end{aligned} \quad (\text{B21})$$

c. 1D case

For one dimension we have instead of Eq. (B7)

$$\int \frac{dp}{(2\pi)} F' G(p) = m \int \frac{dp}{(2\pi)} F \partial_p \left(\frac{G(p)}{p} \right), \quad (\text{B22})$$

which applied to Eq. (B5) yields

$$\begin{aligned} \Pi_0(\omega) &= \frac{q^2}{3m\omega^2} n - \frac{q^4}{60m^2\omega^2} \partial_\mu n + \frac{6q^4}{5m^2\omega^4} E, \\ \tilde{\Pi}_2(\omega) &= \frac{2q^2}{3\omega^2} E - \frac{q^4}{60m\omega^2} n + \frac{4q^4}{5m\omega^4} E_2, \\ \tilde{\Pi}_4(\omega) &= \frac{4mq^2}{3\omega^2} E_2 - \frac{q^4}{10\omega^2} E + \frac{24q^4}{25\omega^4} E_3. \end{aligned} \quad (\text{B23})$$

The static case is

$$\begin{aligned} \Pi_0(0) &= -\partial_\mu n + \frac{q^2}{12m} \partial_\mu^2 n, \\ \tilde{\Pi}_2(0) &= -mn + \frac{q^2}{12} \partial_\mu n, \\ \tilde{\Pi}_4(0) &= -6m^2 E + \frac{mq^2}{4} n. \end{aligned} \quad (\text{B24})$$

The occurring moments read here

$$\begin{aligned} n = \langle 1 \rangle &= \frac{s}{4\lambda} f_{1/2}, \\ E = \left\langle \frac{p^2}{2m} \right\rangle &= \frac{1}{2} \int^\mu d\mu' n = \frac{1}{8\beta} \frac{s}{\lambda} f_{3/2}, \\ E_2 = \left\langle \left(\frac{p^2}{2m} \right)^2 \right\rangle &= \frac{3}{2} \int^\mu d\mu' E = \frac{3}{16\beta^2} \frac{s}{\lambda} f_{5/2}, \\ E_3 = \left\langle \left(\frac{p^2}{2m} \right)^3 \right\rangle &= \frac{5}{2} \int^\mu d\mu' E_2 = \frac{15}{32\beta^3} \frac{s}{\lambda} f_{7/2}. \end{aligned} \quad (\text{B25})$$

2. Large-frequency limit

The large-frequency limit can be given analogously to the foregoing section. We restrict here to the expansion for 3D,

$$\Pi_0(\omega) = \frac{q^2}{m\omega^2} n + \frac{2q^4}{m^2\omega^4} E + \frac{q^6}{4m^3\omega^4} n + o\left(\frac{1}{\omega^6}\right). \quad (\text{B26})$$

Please note the difference from the large-wavelength expansion (B8). The corresponding higher-order correlation functions are completely analogously given by the methods of the foregoing section. With Eqs. (B4) and (B3), one gets

$$\bar{\Pi}_2(\omega) = \frac{4q^2}{3\omega^2}E + \frac{8q^4}{5m\omega^4}E_2 + \frac{q^6}{3m^2\omega^4}E + o\left(\frac{1}{\omega^6}\right),$$

$$\bar{\Pi}_4(\omega) = \frac{32mq^2}{15\omega^2}E_2 + \frac{64q^4}{35\omega^4}E_3 + \frac{8q^6}{15m\omega^4}E_2 + o\left(\frac{1}{\omega^6}\right). \quad (\text{B27})$$

PERTURBATION THEORY AND FREQUENCY SUM RULES FOR ONE, TWO, AND THREE DIMENSIONS

The external potential is adiabatically switched on,

$$V^{\text{ext}}(r,t) = V(r)e^{0t}\Theta(-t), \quad (\text{C1})$$

and induces a time-dependent change in the Hamiltonian operator,

$$\delta\hat{H}(t) = - \int dr \hat{n}(r,t) V^{\text{ext}}(r,t). \quad (\text{C2})$$

The variation of the density matrix operator $\hat{\rho}(t) = \hat{\rho} + \delta\hat{\rho}(t)$ can be found from the linearized van Neumann equation as

$$\delta\hat{\rho}(t) = -i \int_{-\infty}^t [\delta\hat{H}, \hat{\rho}_0], \quad (\text{C3})$$

where it has been assumed that the perturbation is conserving symmetries of the equilibrium Hamiltonian, $[\hat{H}_0, \delta\hat{\rho}] = 0$.

The variation of the density expectation value $\delta n = \text{Tr} \delta\rho \hat{n}$ is consequently

$$\delta n(r,t) = i \int_{-\infty}^t dt' \int dr' V(r',t') \langle [\hat{n}(r,t), \hat{n}(r',t')] \rangle. \quad (\text{C4})$$

Since in equilibrium the commutator is only dependent on the difference of coordinates and times we can define

$$\begin{aligned} & -2 \text{Im} \chi(q, \omega) \\ &= \int dt e^{i\omega(t-t')} \int dr dr' e^{-iq(r-r')} \langle [\hat{n}(r,t), \hat{n}(r',t')] \rangle, \end{aligned} \quad (\text{C5})$$

from which we obtain the Fourier transform of Eq. (C4) to

$$\delta n(q, \omega) = V^{\text{ext}}(q, \omega) \int \frac{d\bar{\omega}}{\pi} \frac{\text{Im} \chi(q, \bar{\omega})}{\bar{\omega} - \omega - i0}, \quad (\text{C6})$$

where $V^{\text{ext}}(q, \omega) = V^{\text{ext}}(q)/(0 + i\omega)$. This is of course identical with Eq. (1).

3. Sum rules

Now one can derive the first- and second-order sum rules of the imaginary part of the response function (C5). Therefore we generalize the definition (C5) to nonequilibrium and finite systems,

$$\begin{aligned} \text{Im} \chi(q, \omega, R, t) &= -\frac{1}{2} \int d\tau e^{i\omega\tau} \int dr e^{-iqr} \langle [\hat{n}(R+r/2, t \\ &+ \tau/2), \hat{n}(R-r/2, t - \tau/2)] \rangle. \end{aligned} \quad (\text{C7})$$

Higher-order moments can be expressed by correlation functions as well.⁵⁶ Here we restrict to the lowest two orders and rederive it in conventional way.

If we assume further equilibrium but finite systems, we can define an averaged response by applying spatial averaging $\int dR/V$ to Eq. (C7), such that we obtain

$$\text{Im} \chi(q, \omega) = -\frac{1}{2V} \int d\tau e^{i\omega\tau} \langle [\hat{n}(q, t), \hat{n}(-q, 0)] \rangle. \quad (\text{C8})$$

From this expression it is easy to see that the first two frequency sum rules read

$$\int \frac{d\omega}{\pi} \omega \text{Im} \chi(q, \omega) = -\frac{1}{V} \langle [i\partial_t \hat{n}(q, t)|_{t=0}, \hat{n}(-q, 0)] \rangle, \quad (\text{C9})$$

$$\int \frac{d\omega}{\pi} \omega^3 \text{Im} \chi(q, \omega) = -\frac{1}{V} \langle [(i\partial_t)^3 \hat{n}(q, t)|_{t=0}, \hat{n}(-q, 0)] \rangle.$$

Using the Heisenberg equation $i\partial_t \hat{n} = [\hat{n}, \hat{H}]$ and

$$\begin{aligned} \hat{H} &= \int \frac{dp}{(2\pi)^D} \frac{p^2}{2m} \hat{a}_p^\dagger \hat{a}_p \\ &+ \frac{1}{2} \int \frac{dp dp_1 dp_2}{(2\pi)^{3D}} V_p \hat{a}_p^\dagger \hat{a}_{p_1}^\dagger \hat{a}_{p_2}^\dagger \hat{a}_{p_2+p} \hat{a}_{p_1-p}, \\ \hat{n}_q &= \int \frac{dp}{(2\pi)^D} \hat{a}_p^\dagger \hat{a}_{p+q}, \end{aligned} \quad (\text{C10})$$

we can express the sum rules (C9) as

$$\begin{aligned} \int \frac{d\omega}{\pi} \omega \text{Im} \chi(q, \omega) &= \frac{1}{V} \langle [q\hat{j}_q, \hat{n}_{-q}] \rangle, \\ \int \frac{d\omega}{\pi} \omega^3 \text{Im} \chi(q, \omega) &= -\frac{1}{V} \langle [q\hat{j}_q, [q\hat{j}_{-q}, \hat{H}]] \rangle, \end{aligned} \quad (\text{C11})$$

where the divergence of the current operator reads

$$q\hat{j}_q = \int \frac{dp}{(2\pi)^D} \frac{2pq + q^2}{2m} \hat{a}_p^\dagger \hat{a}_{p+q}. \quad (\text{C12})$$

Performing the last commutators, one obtains finally

$$\int \frac{d\omega}{\pi} \omega \text{Im} \chi(q, \omega) = \frac{q^2}{m} \frac{\langle \hat{n}_{q=0} \rangle}{V} = n \frac{q^2}{m} \quad (\text{C13})$$

and

$$\begin{aligned} & \int \frac{d\omega}{\pi} \omega^3 \text{Im} \chi(q, \omega) \\ &= \frac{nq^6}{4m^3} + \frac{3q^2}{m^3V} \int \frac{dp}{(2\pi)^D} (pq)^2 \langle \hat{a}_p^\dagger \hat{a}_p \rangle \\ & \times \frac{1}{m^2V} \int \frac{dp}{(2\pi)^D} V_p \\ & \times \left\{ (pq)^2 \int \frac{dp_1 dp_2}{(2\pi)^{2D}} \hat{a}_{p_1}^\dagger \hat{a}_{p_2}^\dagger \hat{a}_{p_2+p+q} \hat{a}_{p_1-p-q} \right. \\ & \left. - [(pq)^2 - q^2(pq)] \int \frac{dp_1 dp_2}{(2\pi)^{2D}} \hat{a}_{p_1}^\dagger \hat{a}_{p_2}^\dagger \hat{a}_{p_2-p} \hat{a}_{p_1+p} \right\}. \end{aligned} \quad (\text{C14})$$

Since we had symmetric expressions, $\phi(p) = \phi(-p)$, the second term leads just to kinetic-energy density

$$\begin{aligned} & \frac{3q^2}{m^3V} \int \frac{dp}{(2\pi)^D} (pq)^2 \langle \hat{a}_p^\dagger \hat{a}_p \rangle \\ &= \frac{2q^4}{m^2V} \int \frac{dp}{(2\pi)^D} \frac{p^2}{2m} \langle \hat{a}_p^\dagger \hat{a}_p \rangle \begin{cases} 3 & \text{for 1D} \\ 1 & \text{for 2D,3D} \end{cases} \\ &= \frac{2q^4E}{m^2} \begin{cases} 3 & \text{for 1D} \\ 1 & \text{for 2D,3D.} \end{cases} \end{aligned} \quad (\text{C15})$$

Now we are going to express the last four creation and annihilation operators using the structure function itself. Therefore we use the definition of the pair-correlation function

$$\langle \hat{a}_{r_1}^\dagger \hat{a}_{r_2}^\dagger \hat{a}_{r_2} \hat{a}_{r_1} \rangle = g_r n(r_1) n(r_2). \quad (\text{C16})$$

Applying the spatial averaging $\int dR/V$, where $R = (r_1 + r_2)/2$ and Fourier transforming the difference $r_1 - r_2$ into q , we obtain

$$\begin{aligned} & \int \frac{dp_1 dp_2}{(2\pi)^{2D} V} \hat{a}_{p_1}^\dagger \hat{a}_{p_2}^\dagger \hat{a}_{p_2+q} \hat{a}_{p_1-q} \\ &= \int dr e^{-i(rq)} g_r \int \frac{dR}{V} n(R+r/2) n(R-r/2) \\ &= n^2 \int dr e^{-i(rq)} (g_r - 1) + n^2 (2\pi)^3 \delta(q) \\ &= n(S_q - 1) + n^2 (2\pi)^3 \delta(q), \end{aligned} \quad (\text{C17})$$

where we neglected spatial gradients in the density and used Eq. (11) for the last step. Using Eq. (C17) in Eq. (C14) we obtain finally

$$\begin{aligned} & \int \frac{d\omega}{\pi} \omega^3 \text{Im} \chi(q, \omega) \\ &= \frac{nq^6}{4m^3} + \frac{2q^2E}{m^2} \begin{cases} 3 & \text{for 1D} \\ 1 & \text{for 2D,3D} \end{cases} \\ & \quad - \frac{n^2}{m^2} q^4 V_q \left(\tilde{I}(q) + \begin{cases} \tilde{I}_1(q) & \text{for 1D} \\ 0 & \text{for 2D,3D} \end{cases} \right) \end{aligned} \quad (\text{C18})$$

with Eq. (26),

$$\tilde{I}(q) = -\frac{1}{n} \int \frac{dk}{(2\pi)^D} (S_{k-q} - S_k + n \delta_{k,q} - n \delta_{k,0}) \frac{(kq)^2}{q^4} \frac{V_k}{V_q}, \quad (\text{C19})$$

where we understand $\delta_k = (2\pi)^3 \delta(k)$. For the one-dimensional case an extra term appears,

$$\tilde{I}_1(q) = \frac{1}{n} \int \frac{dk}{(2\pi)} (S_{k-1+n} \delta_{k,0}) \frac{kV_k}{qV_q}. \quad (\text{C20})$$

In the following we restrict to the required formulas for the three-dimensional case. One can Fourier transform

$$\tilde{I}(q) = - \int dr g_r [1 - \cos(qr)] \frac{(q\partial_r)^2 V_r}{q^4 V_q}, \quad (\text{C21})$$

which was first given by Puff.⁸ This correct form leads unavoidably to the appearance of the δ_p terms in Eq. (C19), very often overseen in later papers. For asymptotic expansions, however, we have to be careful that $g_r - 1$ is the object that renders spatial integrals finite. Therefore the δ_p terms in Eq. (C19) have to be considered separately,

$$-\frac{1}{n} \int \frac{dk}{(2\pi)^3} (n \delta_{k,q} - n \delta_{k,0}) \frac{(kq)^2}{q^4} \frac{V_k}{V_q} = -1, \quad (\text{C22})$$

such that we obtain instead of Eq. (C21),

$$\tilde{I}(q) = - \int dr (g_r - 1) [1 - \cos(qr)] \frac{(q\partial_r)^2 V_r}{q^4 V_q} - 1. \quad (\text{C23})$$

For Coulomb potentials we can further simplify

$$\tilde{I}(q) = -2 \int_0^\infty \frac{dr}{r} (g_r - 1) j_2(qr) - 1 \quad (\text{C24})$$

with the spherical Bessel function $j_2(x)$. From this expression one sees the small-wave-vector limit

$$\begin{aligned} \tilde{I}(q) &= -\frac{2q^2}{15} \int_0^\infty dr r (g_r - 1) - 1 + o(q^4) \\ &= \frac{2}{5} \frac{q^2}{k_f^2} \gamma - 1 + o(q^4), \end{aligned} \quad (\text{C25})$$

where we have used Eq. (11) and definition (9). The long-wave-vector limit takes the form

$$\begin{aligned} \tilde{I}(q) &= -2 \int_0^\infty \frac{dx}{x} (g_{x/q} - 1) j_2(x) - 1 \\ &= -2(g_0 - 1) \int_0^\infty \frac{dx}{x} j_2(x) - 1 + o(1/q^2) \\ &= \frac{2}{3} (1 - g_0) - 1 + o(1/q^2). \end{aligned} \quad (\text{C26})$$

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